

Abstract No. napo672

Crystal Structure of a DNA Duplex in Two, Statistically Equivalent, Conformations

A. Napoli, S. Chen, B. Benoff, S. Bodige, and H. Berman (Rutgers U.)

Beamline(s): X12C

Introduction: The crystal structure of duplex DNA containing the sequence 5'-GCGTGGGCAC-3' has been solved to 1.9 Å resolution. The sequence is the recognition sequence for a variant of Zif268, a zinc finger DNA binding protein.

Results: The decamer crystallizes in space group $P6_122$ with cell constants of $a=38.23$ $c=76.15$. The DNA exists in the crystal lattice in two distinct, statistically equivalent orientations. The existence of this statistical disorder was proven by an $fo-fc$ electron density map. Although a bromo-uridine derivative contained only two bromine atoms in the duplex structure, the difference map clearly identified the location of four bromine sites. A model with both orientations, each with 50% occupancy, is being used for refinement.

Conclusions: Comparison of this DNA structure to the protein-DNA complex structure is impossible because the DNA is A-form in this crystal. The A-form structure may be a result of the crystallization conditions, which contain Cobalt Hexamine. Based on this and other A-form DNA structures, the high GC content may also play a role in the tendency towards the A-form conformation. Finally, the fact that this lattice cannot differentiate the direction of this DNA sequence suggests that the lattice could accommodate several variations of similar sequences in the same lattice.

Reference:

A.D. DiGabriele, T.A. Steitz, "A DNA Dodecamer Containing an Adenine Tract Crystallizes in a Unique Lattice and Exhibits a New Bend," *J Mol Biol*, Jun 20; 231(4):1024-39, 1993.